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Progress Report on Collaborative Research on the Development of Chelators for a Surface Decontamination Foam

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Progress Report on Collaborative Research on the Development of Chelators for a Surface Decontamination Foam - June 30th, 2009 -



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Cs, Sr & Co – Chelate Models

Running the models:

Chemical thermodynamic modeling using data from the NIST Critical Stability Constant Database v46.

No data available for Cs DTPA and Cs NTA.

Not kinetic – assumes complete reaction.

1 micromolar metal solutions.

1 micromolar to 1 molar chelator solution.

Titrate pH.

Some models did not converge at high chelate concentration.



Cs, Sr & Co – Chelate Models

Data Caveats:

Data show optimum pH and chelate concentration for maximum chelator efficiency.

Models do not show speciation....

EDTA binds lots of metals effectively (i.e. non-specific).

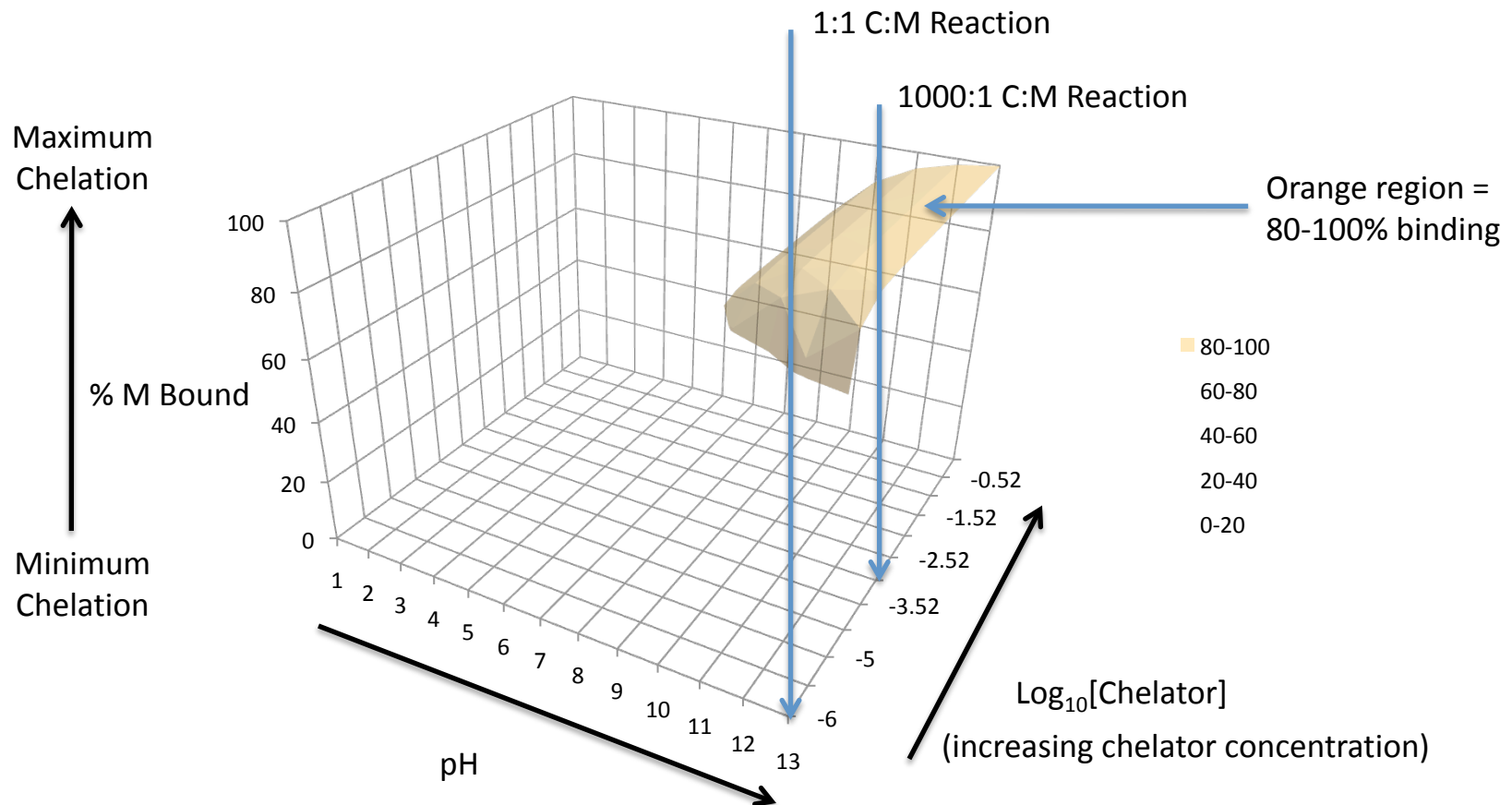
EDTA shows >60% efficiency for Cs at high pH, but in the real world (with natural background levels of other metals), EDTA will never bind Cs efficiently.

However, it is possible to vary pH to alter EDTA specificity for Co in a mixture of Sr and Cs....

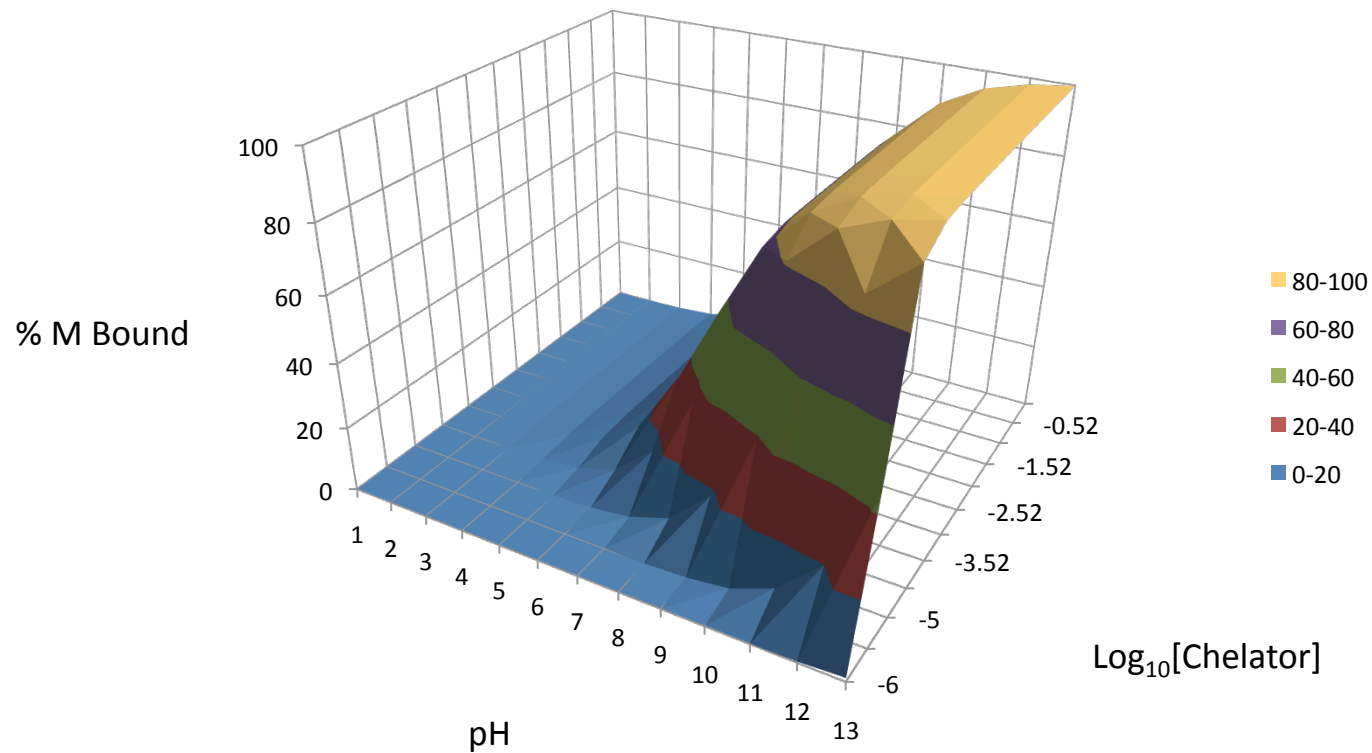
EDTA binds to Co at pH 2-12, Sr at pH 4-12 and poorly to Cs. Therefore, to selectively bind Co, maintain pH <4.



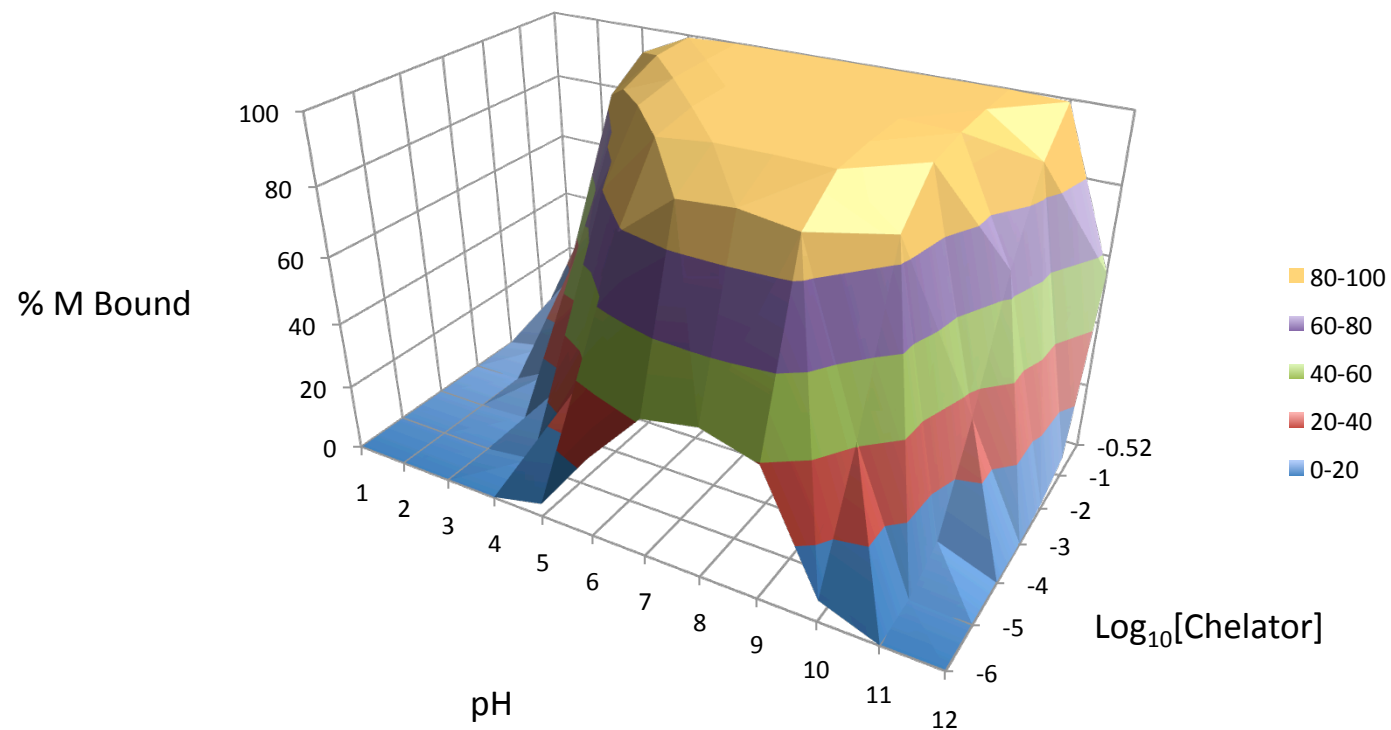
M – Chelate Contours



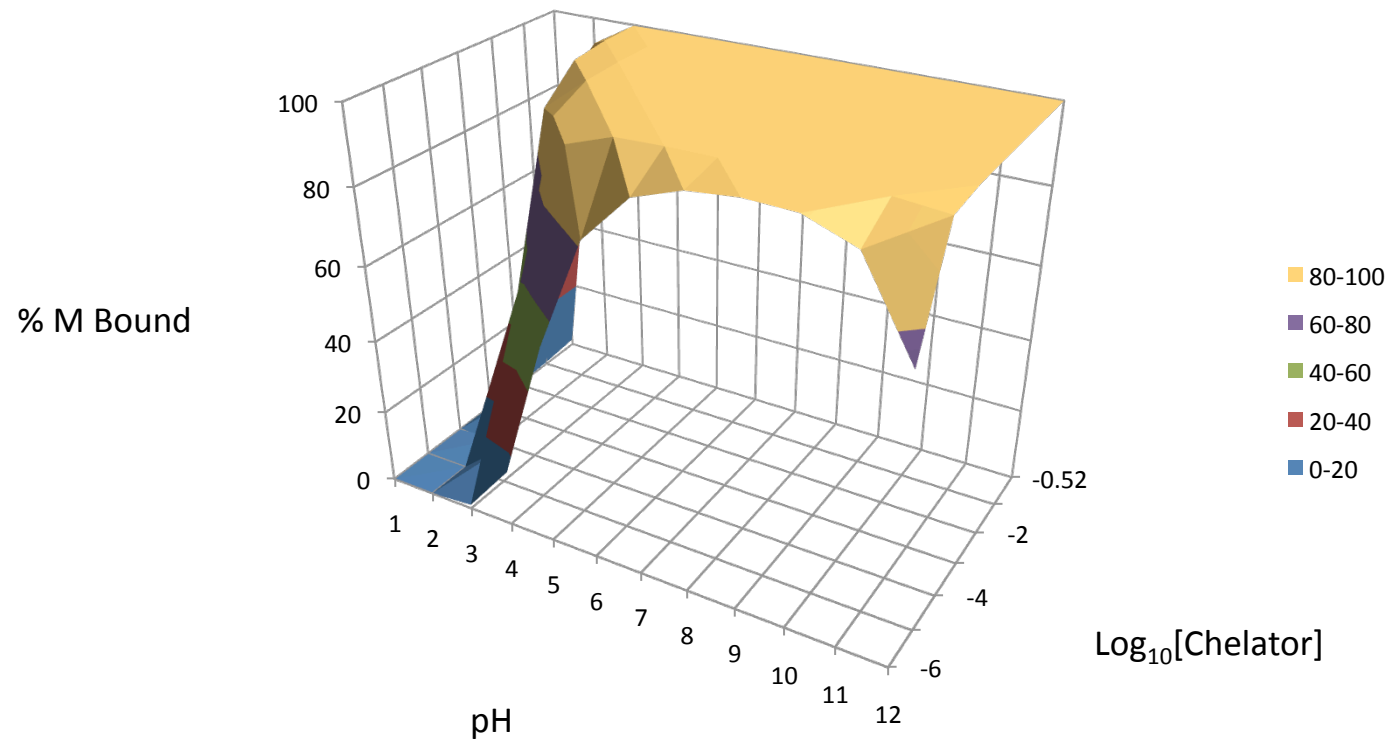
Cs – Prussian Blue



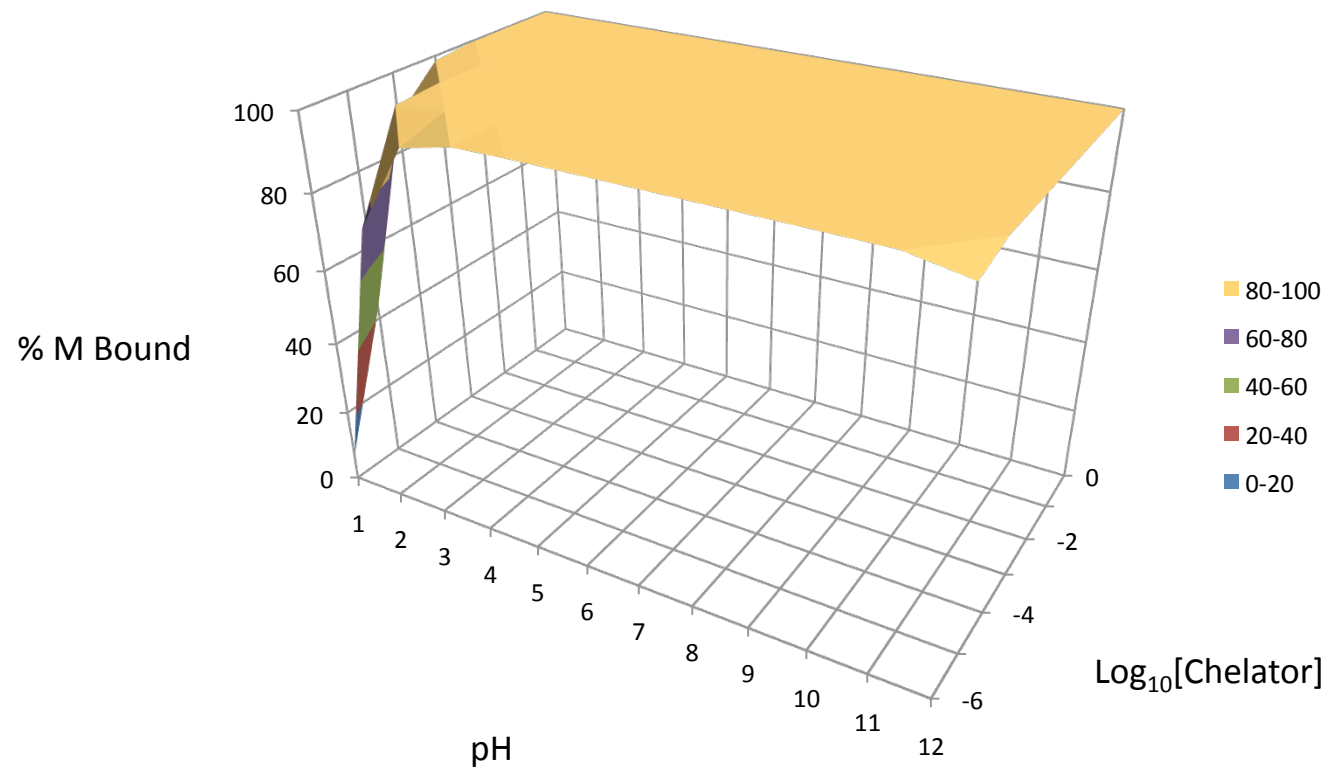
Co – Citrate



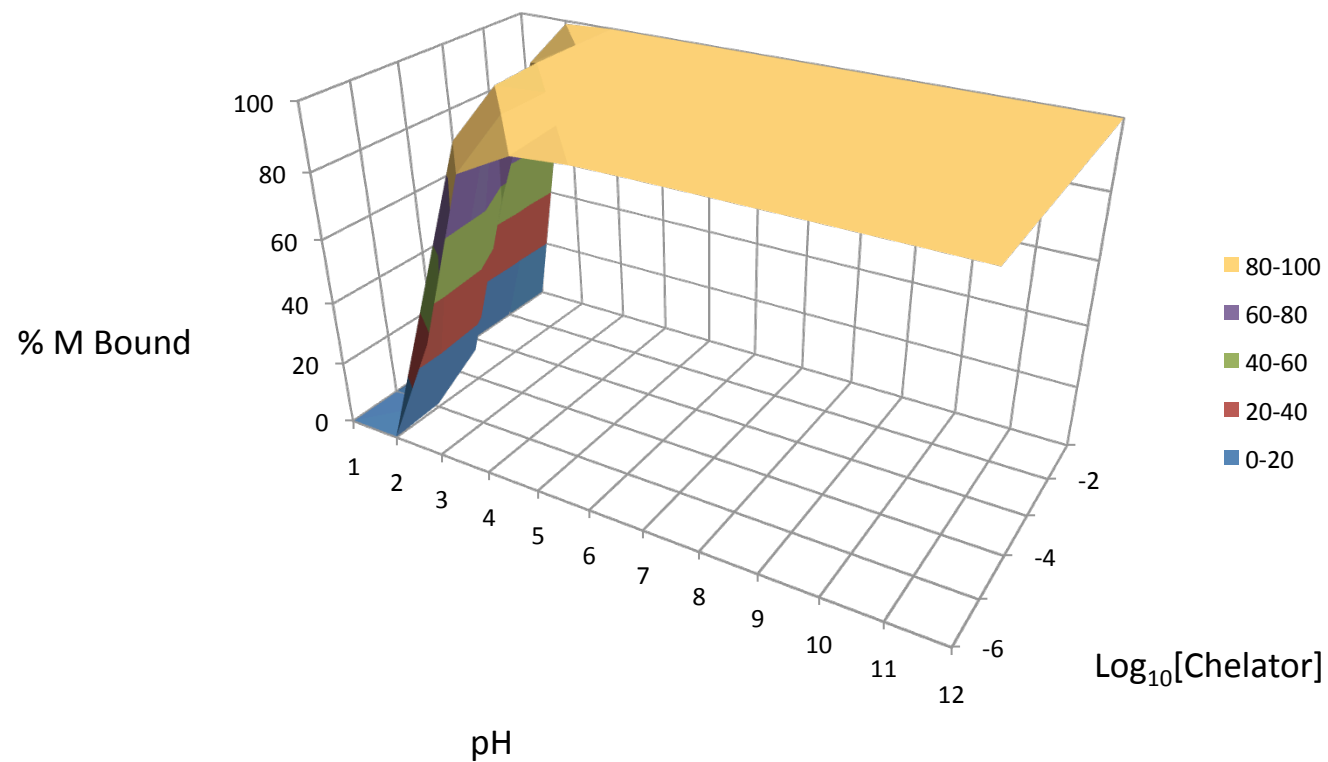
Co – NTA



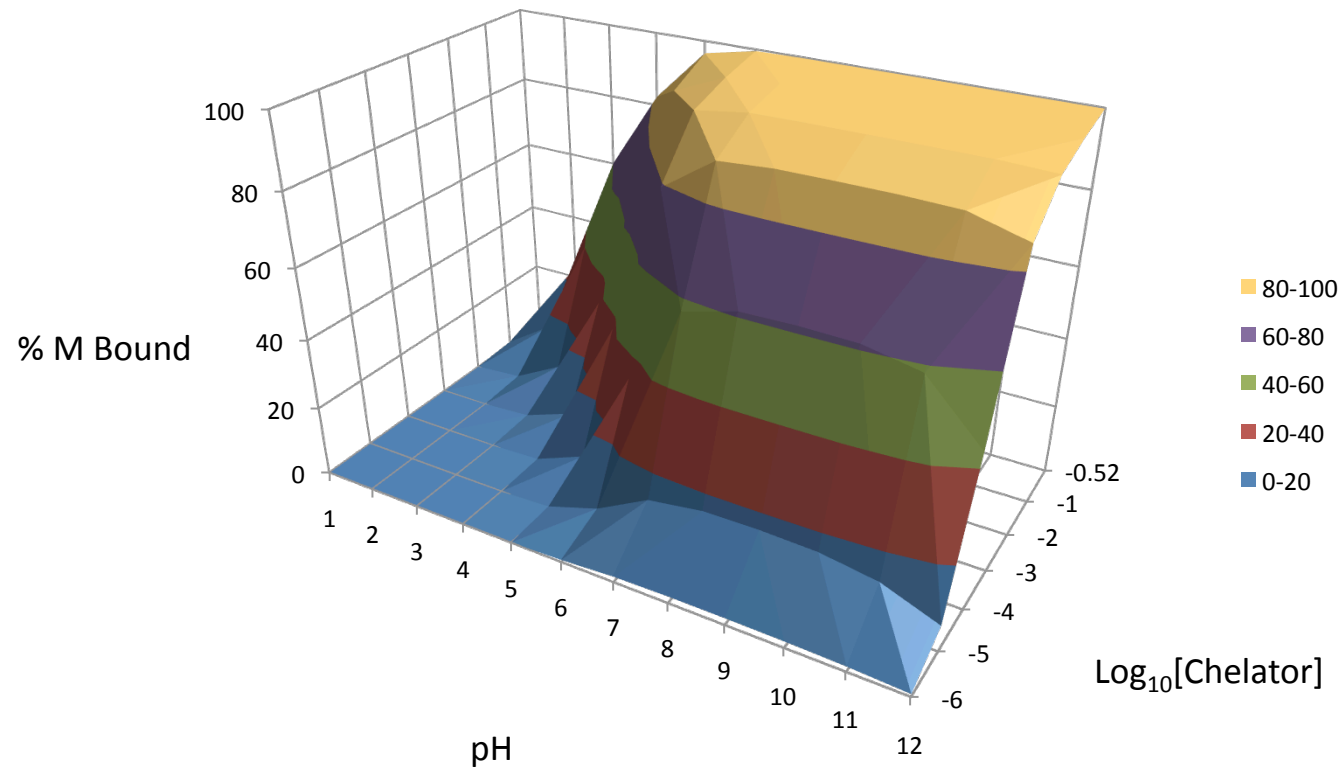
Co – EDTA



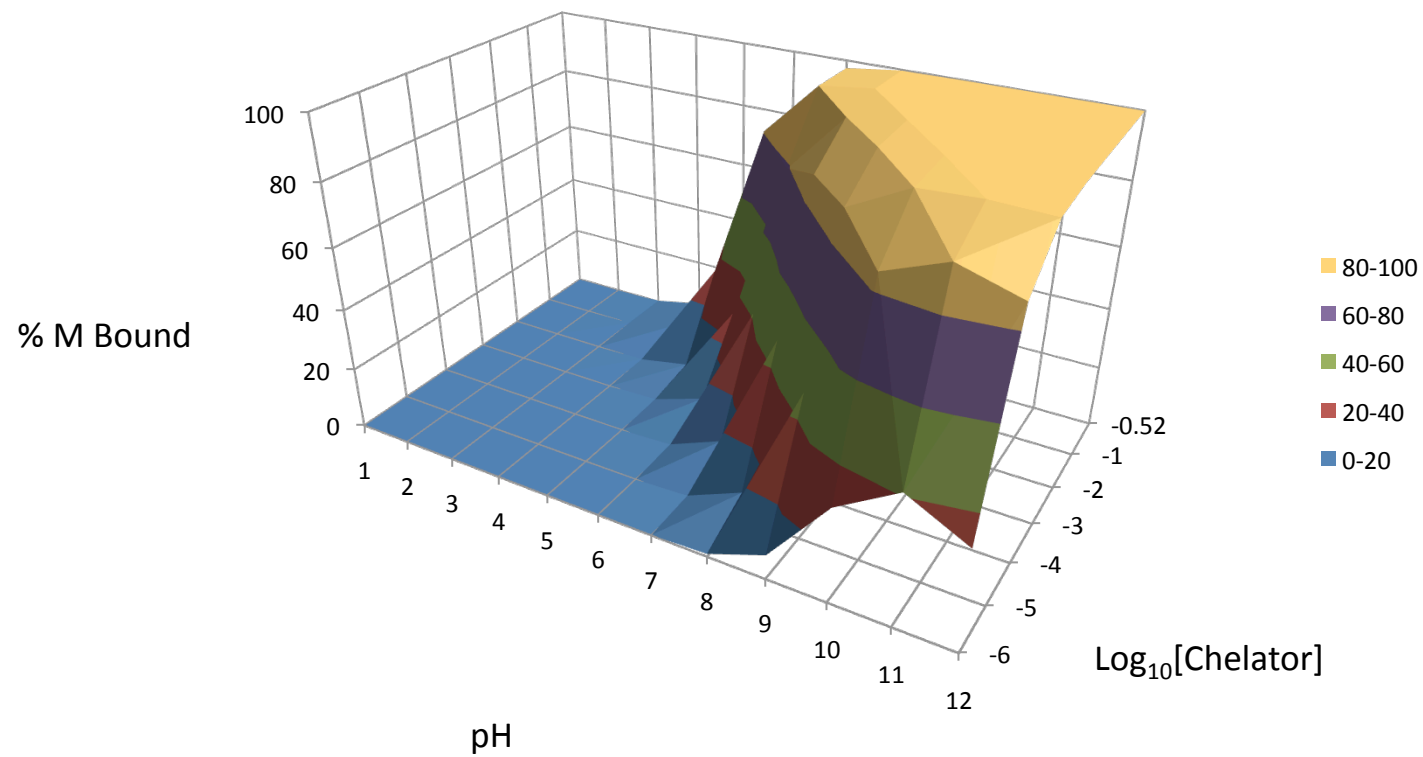
Co – DTPA



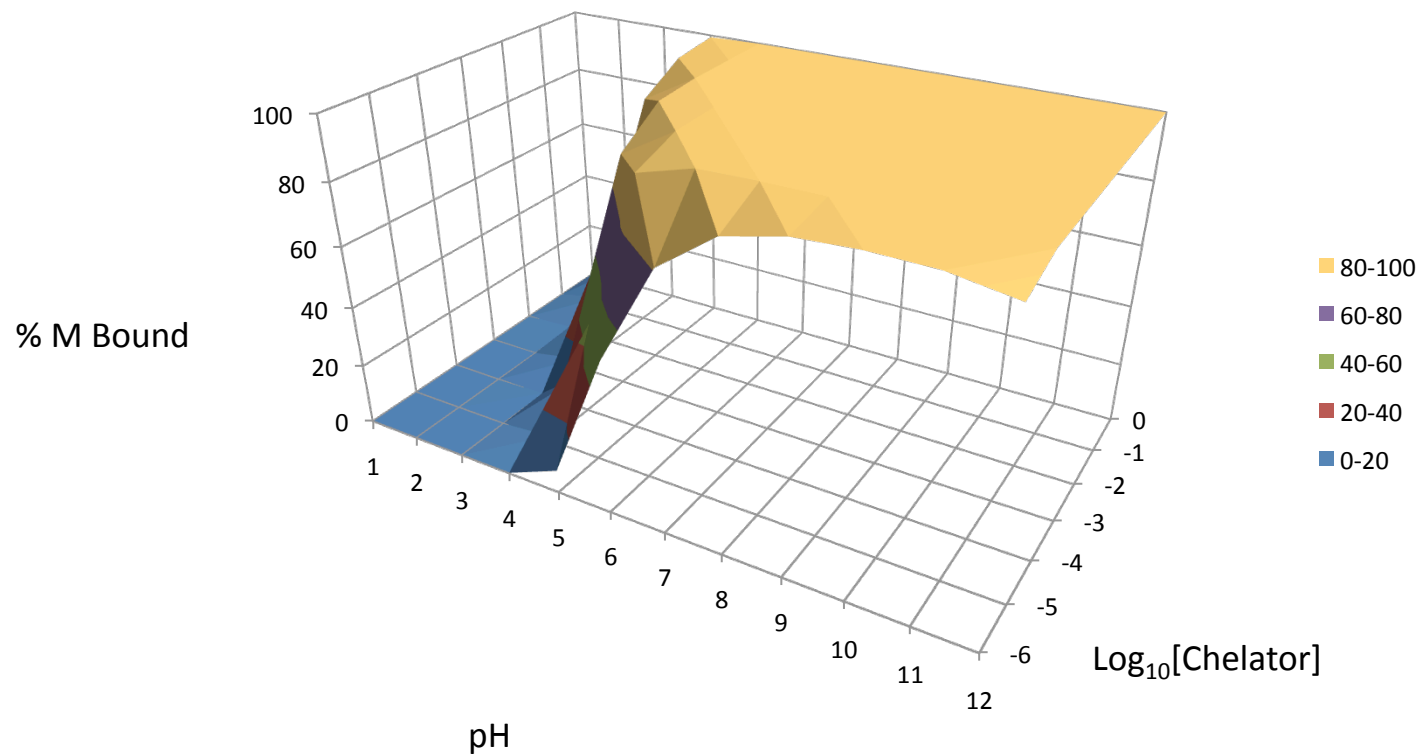
Sr – Citrate



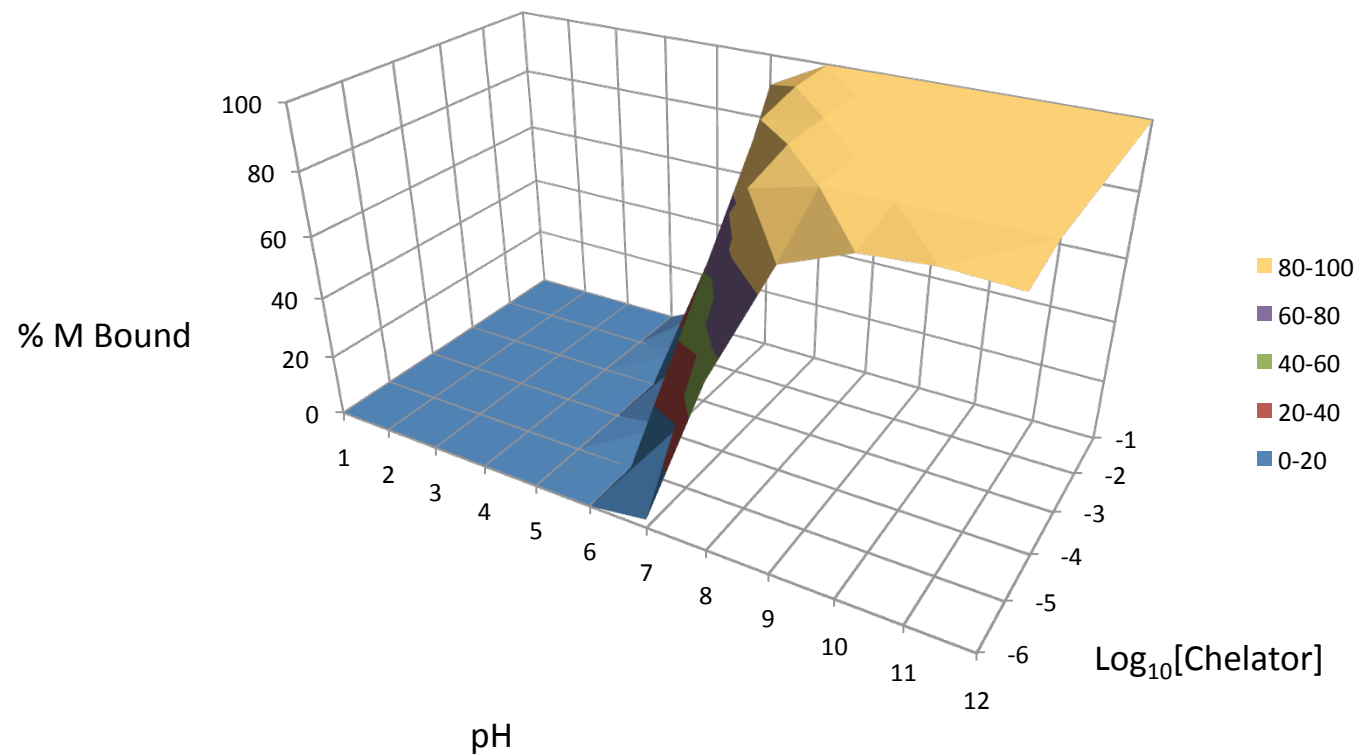
Sr – NTA



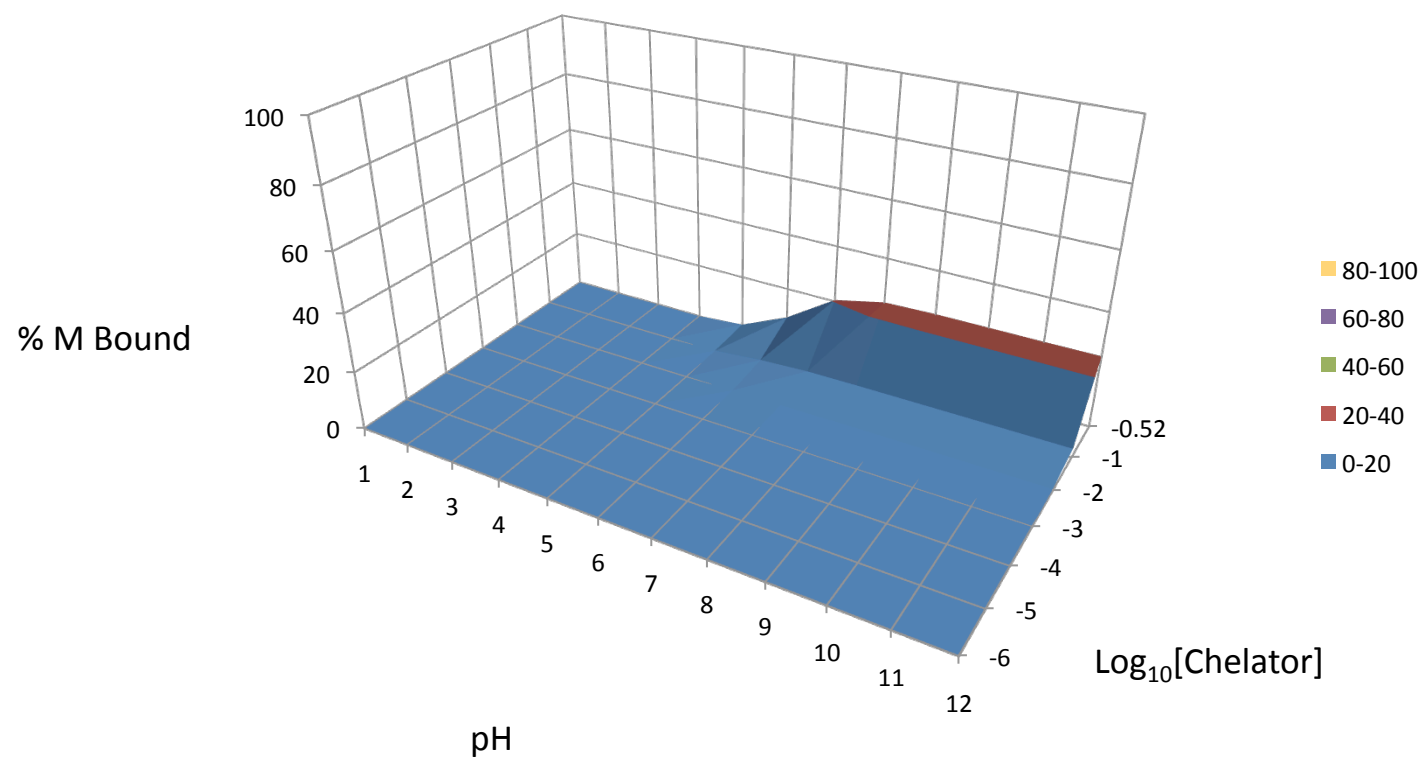
Sr – EDTA



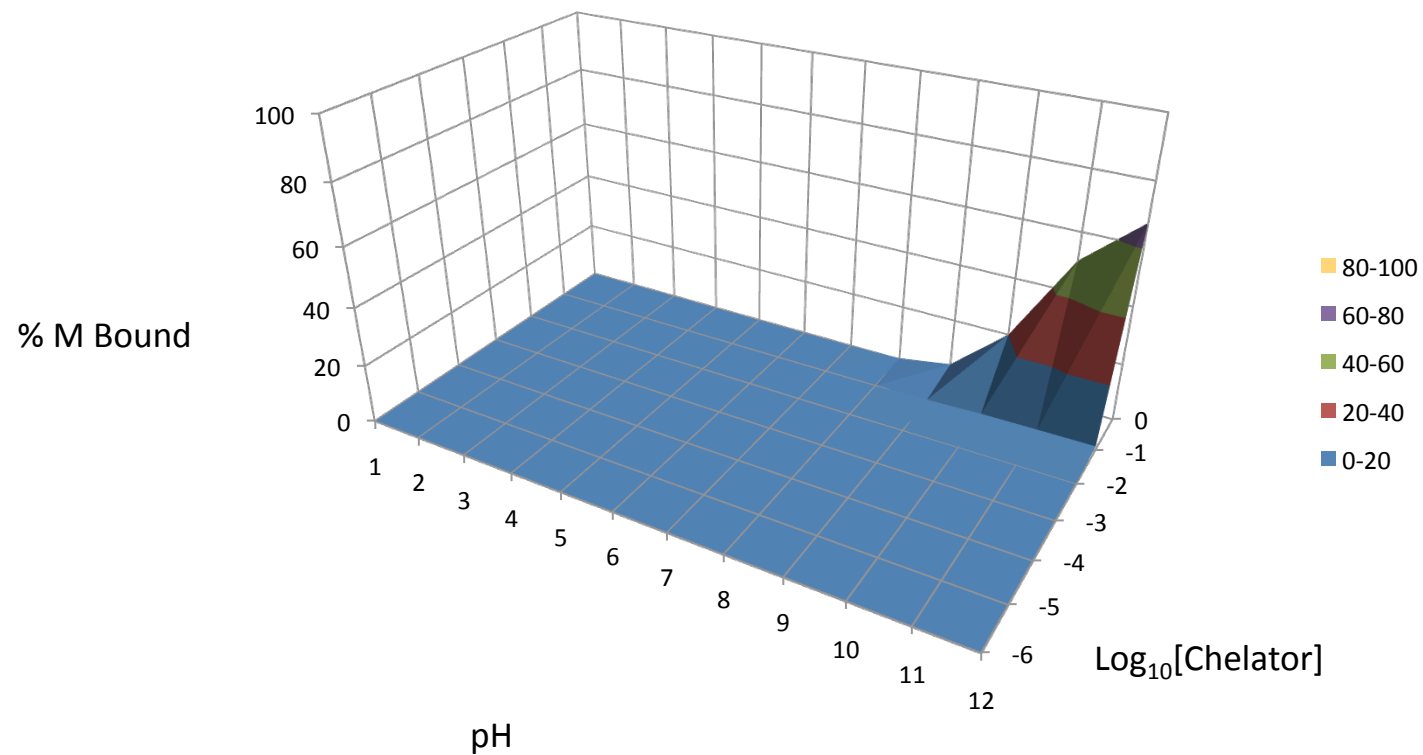
Sr – DTPA



Cs – Citrate



Cs – EDTA



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